

N-(3-Methoxybenzoyl)-2-methylbenzenesulfonamide

S. Sreenivasa,^a D Darshan,^b M. Prakash Shet,^c
N. R. Mohan,^a Vijith Kumar^d and P. A. Suchetan^{c*}

^aDepartment of Studies and Research in Chemistry, Tumkur University, Tumkur, Karnataka 572 103, India, ^bUniversity College of Science, Tumkur University, Tumkur, India, ^cDepartment of Studies and Research in Chemistry, U.C.S., Tumkur University, Tumkur, Karnataka 572 103, India, and ^dSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India
Correspondence e-mail: pasuchetan@yahoo.co.in

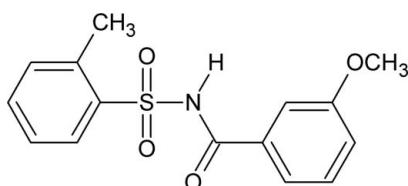
Received 29 June 2013; accepted 4 July 2013

Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$; R factor = 0.045; wR factor = 0.118; data-to-parameter ratio = 13.1.

In the title compound, $\text{C}_{15}\text{H}_{15}\text{NO}_4\text{S}$, the dihedral angle between the methyl- and methoxy-substituted benzene rings is $88.99(12)^\circ$. An intramolecular C—H···O hydrogen bond occurs. In the crystal, adjacent molecules form inversion-related dimers through strong N—H···O hydrogen bonds, generating $R_2^2(8)$ loops. The dimers are further connected through C—H···O interactions that form $C(8)$ chains parallel to (001). Molecules are also connected through other C—H···O hydrogen bonds along the b axis, forming additional $C(8)$ chains. Two aromatic π – π stacking interactions [centroid–centroid separations = $3.6150(1)$ and $3.6837(1)\text{ \AA}$] generate a three-dimensional architecture.

Related literature

For similar structures, see: Gowda *et al.* (2010); Suchetan *et al.* (2010, 2011).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}_4\text{S}$
 $M_r = 305.34$
Monoclinic, $C2/c$

$a = 26.713(5)\text{ \AA}$
 $b = 7.3717(4)\text{ \AA}$
 $c = 19.636(3)\text{ \AA}$

$\beta = 131.21(3)^\circ$
 $V = 2908.7(7)\text{ \AA}^3$
 $Z = 8$
Mo $K\alpha$ radiation

$\mu = 0.24\text{ mm}^{-1}$
 $T = 293\text{ K}$
 $0.33 \times 0.27 \times 0.22\text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer
5294 measured reflections
2558 independent reflections
1970 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.118$
 $S = 1.04$
2558 reflections
196 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.19\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.35\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots\cdot A$ | $D\cdots\cdot A$ | $D-\text{H}\cdots\cdot A$ |
|----------------------------|--------------|-------------------------|------------------|---------------------------|
| N1—H N1—O2 ⁱ | 0.80 (3) | 2.15 (4) | 2.929 (4) | 166 |
| C3—H3—O3 ⁱⁱ | 0.93 | 2.60 | 3.463 (3) | 155 |
| C10—H10—O2 ⁱ | 0.93 | 2.60 | 3.404 (3) | 145 |
| C15—H15B—O3 ⁱⁱⁱ | 0.96 | 2.36 | 3.323 (3) | 178 |
| C6—H6—O1 | 0.93 | 2.46 | 2.861 (4) | 106 |

Symmetry codes: (i) $-x, y, -z + \frac{1}{2}$; (ii) $x, y - 1, z$; (iii) $x, -y + 2, z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APPEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor T. N. Guru Row, Soild State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, for his help and valuable suggestions. PAS and MPS thank the University Grants Commission (UGC), India, for financial support under its Minor Research Project scheme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5340).

References

- Bruker (2009). *APPEX2, SADABS, SAINT-Plus* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2010). *Acta Cryst. E66*, o433.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst. 41*, 466–470.
- Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.
- Suchetan, P. A., Foro, S. & Gowda, B. T. (2011). *Acta Cryst. E67*, o3489.
- Suchetan, P. A., Gowda, B. T., Foro, S. & Fuess, H. (2010). *Acta Cryst. E66*, o1024.

supplementary materials

Acta Cryst. (2013). E69, o1232 [doi:10.1107/S1600536813018539]

N-(3-Methoxybenzoyl)-2-methylbenzenesulfonamide

S. Sreenivasa, D Darshan, M. Prakash Shet, N. R. Mohan, Vijith Kumar and P. A. Suchetan

Comment

As a part of our continued efforts to study the crystal structures of N-(aryloyl)-arylsulfonamides (Suchetan *et al.*, 2010, 2011), we report herein the crystal structure of the title compound (I).

In the title compound, $C_{15}H_{15}NO_4S$, the dihedral angle between the benzene rings is 88.99° . In the molecule, the conformation between the N-H bond and the ortho-methyl group in the sulfonyl benzene ring is *syn*. This is similar to what is observed in N-(benzoyl)-2-methylbenzenesulfonamide (II, Suchetan *et al.*, 2010), N-(3-chlorobenzoyl)-2-methylbenzenesulfonamide (III, Suchetan *et al.*, 2011) and N-(3-methylbenzoyl)-2-methylbenzenesulfonamide (IV, Gowda *et al.*, 2010). Similarly, the conformation between the N-H bond and the meta-methoxy group in the benzoyl ring is *syn*, also similar to the conformation in III (Suchetan *et al.*, 2011) and IV (Gowda *et al.*, 2010).

Adjacent molecules form inversion related dimers through strong $N1-HN1\cdots O2$ hydrogen bonds, Table 1, generating $R^2_2(8)$ loops. The dimers are further connected through intermolecular $C10-H10\cdots O2$ interactions that form $C(8)$ chains parallel to (001). Molecules are also connected through other intermolecular $C15-H15B\cdots O3$ hydrogen bonds along the *b* axis forming additional $C(8)$ chains. Two aromatic $\pi-\pi$ stacking interactions (centroid-centroid separations 3.6150 (1) Å and 3.6837 (1) Å) are also observed.

Experimental

The title compound was prepared by refluxing a mixture of 3-methoxybenzoic acid, 2-methylbenzenesulfonamide and phosphorus oxychloride, $POCl_3$, for 2 h on a water bath. The resultant mixture was cooled and poured into ice cold water. The solid obtained was filtered and washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. The filtered and dried solid was recrystallized to the constant melting point (423 K).

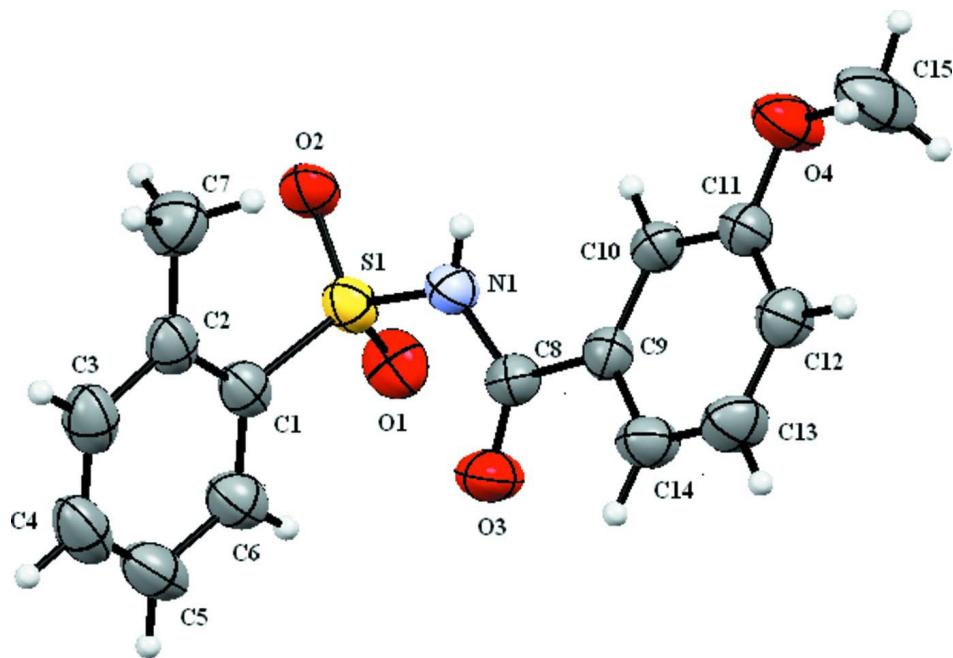
Colorless prisms of (I) were obtained from a slow evaporation of its ethanolic solution at room temperature.

Refinement

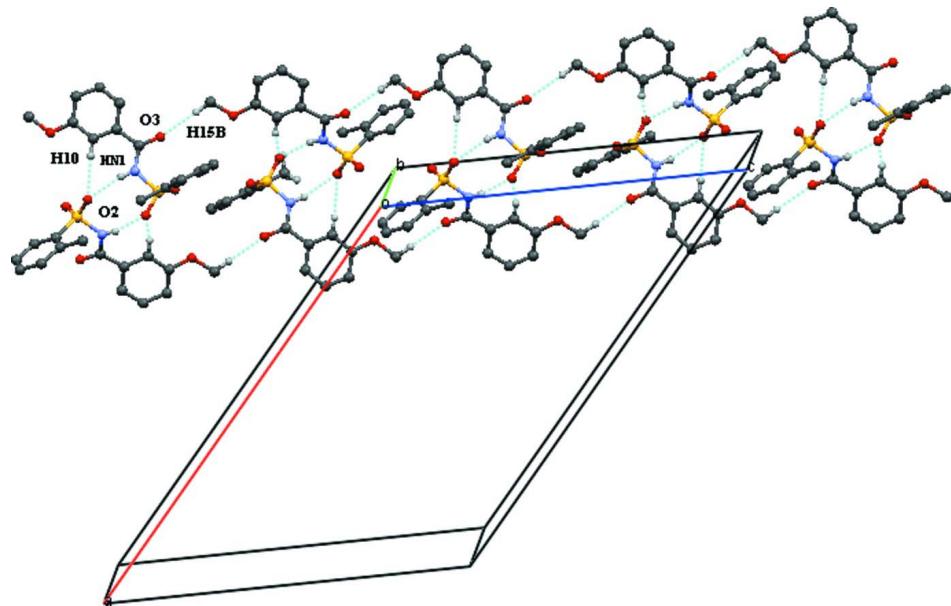
The H atom of the NH group was located in a difference map and later refined freely. The other H atoms were positioned with idealized geometry using a riding model with $C-H = 0.93$ Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Computing details

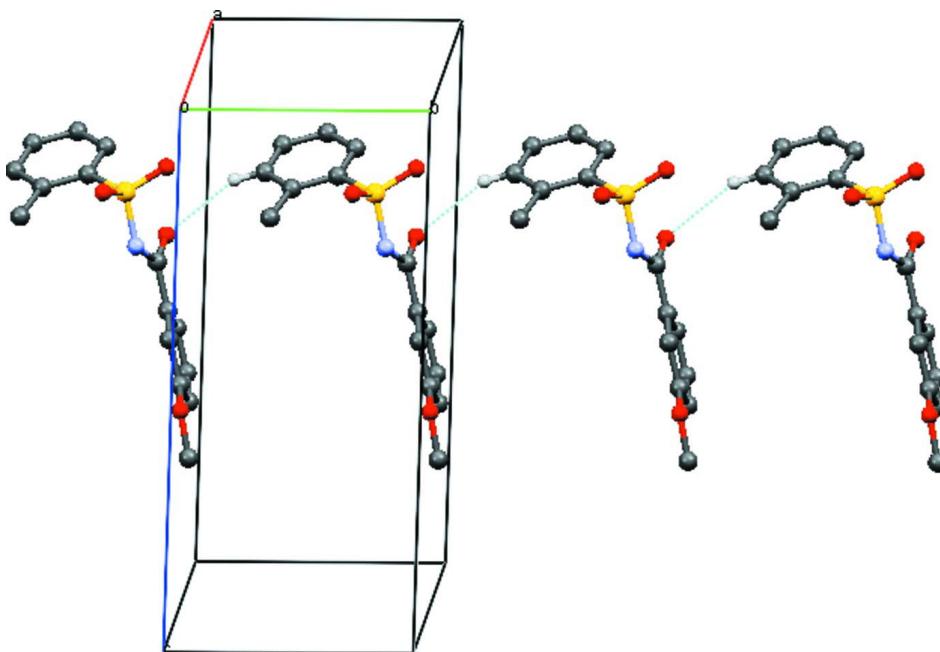
Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

**Figure 1**

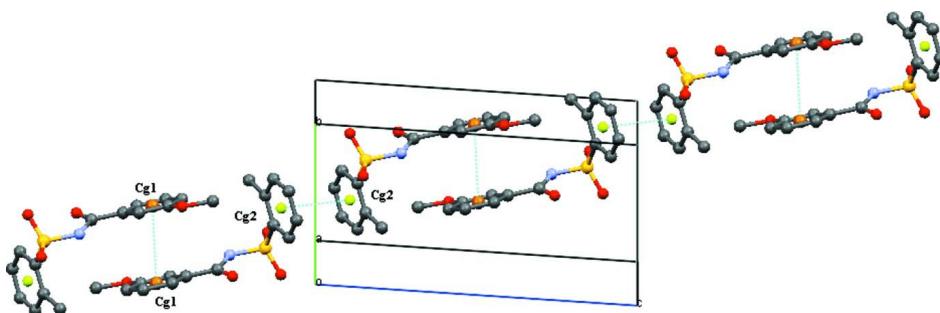
Molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

Molecular packing of (I) with hydrogen bonding shown as dashed lines. Hydrogen atoms bound to carbon are omitted for clarity.

**Figure 3**

Display of C—H···O interactions among molecules along *b* axis forming C(8) chains.

**Figure 4**

Stacking of molecules through $Cg\cdots Cg$ interactions. $Cg1$ and $Cg2$ are the centroids of the carbonyl and sulfonyl bounded benzene rings respectively.

N-(3-Methoxybenzoyl)-2-methylbenzenesulfonamide

Crystal data

$C_{15}H_{15}NO_4S$
 $M_r = 305.34$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
 $a = 26.713 (5)$ Å
 $b = 7.3717 (4)$ Å
 $c = 19.636 (3)$ Å
 $\beta = 131.21 (3)^\circ$
 $V = 2908.7 (7)$ Å³
 $Z = 8$
 $F(000) = 1280$

Prism
 $D_x = 1.394$ Mg m⁻³
Melting point: 423 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1232 reflections
 $\theta = 2.8\text{--}25.0^\circ$
 $\mu = 0.24$ mm⁻¹
 $T = 293$ K
Prism, colourless
 $0.33 \times 0.27 \times 0.22$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
5294 measured reflections
2558 independent reflections

1970 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.8^\circ$
 $h = -31 \rightarrow 31$
 $k = -8 \rightarrow 8$
 $l = -14 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.118$
 $S = 1.04$
2558 reflections
196 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.0171P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|------------|--------------|----------------------------------|
| HN1 | 0.0737 (12) | 0.796 (3) | 0.2976 (17) | 0.055 (8)* |
| C1 | 0.05769 (11) | 0.6312 (3) | 0.13024 (14) | 0.0444 (5) |
| C9 | 0.18751 (12) | 0.9525 (3) | 0.40254 (15) | 0.0425 (5) |
| C10 | 0.16739 (12) | 0.9650 (3) | 0.45194 (16) | 0.0479 (6) |
| H10 | 0.1231 | 0.9451 | 0.4237 | 0.057* |
| C8 | 0.14165 (12) | 0.9088 (3) | 0.30428 (16) | 0.0467 (6) |
| C2 | 0.06638 (11) | 0.4482 (3) | 0.15570 (16) | 0.0488 (6) |
| C6 | 0.07526 (12) | 0.6977 (3) | 0.08233 (16) | 0.0546 (6) |
| H6 | 0.0689 | 0.8195 | 0.0662 | 0.066* |
| C14 | 0.25399 (13) | 0.9826 (3) | 0.44521 (17) | 0.0529 (6) |
| H14 | 0.2678 | 0.9748 | 0.4125 | 0.063* |
| C11 | 0.21314 (12) | 1.0071 (3) | 0.54308 (17) | 0.0496 (6) |
| C13 | 0.29856 (13) | 1.0235 (3) | 0.53520 (18) | 0.0602 (7) |
| H13 | 0.3429 | 1.0430 | 0.5635 | 0.072* |
| C12 | 0.27921 (12) | 1.0365 (3) | 0.58542 (17) | 0.0529 (6) |
| H12 | 0.3102 | 1.0646 | 0.6468 | 0.063* |
| C5 | 0.10253 (13) | 0.5803 (4) | 0.05870 (18) | 0.0653 (7) |

| | | | | |
|------|--------------|-------------|--------------|-------------|
| H5 | 0.1146 | 0.6233 | 0.0267 | 0.078* |
| C4 | 0.11146 (14) | 0.4011 (4) | 0.08281 (18) | 0.0666 (8) |
| H4 | 0.1296 | 0.3227 | 0.0670 | 0.080* |
| C3 | 0.09384 (13) | 0.3358 (3) | 0.13017 (18) | 0.0601 (7) |
| H3 | 0.1004 | 0.2136 | 0.1457 | 0.072* |
| C7 | 0.04728 (14) | 0.3666 (3) | 0.20628 (19) | 0.0651 (7) |
| H7A | 0.0607 | 0.4466 | 0.2543 | 0.098* |
| H7B | 0.0691 | 0.2516 | 0.2312 | 0.098* |
| H7C | -0.0001 | 0.3496 | 0.1655 | 0.098* |
| C15 | 0.23539 (16) | 1.0486 (5) | 0.68140 (19) | 0.0927 (11) |
| H15A | 0.2674 | 0.9521 | 0.7117 | 0.139* |
| H15B | 0.2121 | 1.0546 | 0.7032 | 0.139* |
| H15C | 0.2578 | 1.1616 | 0.6934 | 0.139* |
| O1 | 0.00755 (9) | 0.9515 (2) | 0.10733 (11) | 0.0614 (5) |
| O2 | -0.02956 (7) | 0.7037 (2) | 0.14851 (11) | 0.0527 (4) |
| O3 | 0.15524 (9) | 0.9414 (2) | 0.25752 (12) | 0.0646 (5) |
| O4 | 0.18890 (10) | 1.0151 (3) | 0.58597 (13) | 0.0771 (6) |
| S1 | 0.02251 (3) | 0.78797 (8) | 0.15606 (4) | 0.0461 (2) |
| N1 | 0.08109 (10) | 0.8300 (3) | 0.26647 (13) | 0.0456 (5) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C1 | 0.0325 (12) | 0.0577 (14) | 0.0369 (12) | -0.0007 (11) | 0.0202 (11) | -0.0079 (10) |
| C9 | 0.0428 (13) | 0.0396 (11) | 0.0460 (14) | -0.0036 (10) | 0.0296 (12) | -0.0046 (10) |
| C10 | 0.0408 (14) | 0.0560 (13) | 0.0514 (15) | -0.0117 (11) | 0.0323 (13) | -0.0128 (11) |
| C8 | 0.0477 (15) | 0.0498 (13) | 0.0500 (15) | -0.0079 (11) | 0.0354 (14) | -0.0059 (11) |
| C2 | 0.0370 (13) | 0.0540 (13) | 0.0470 (14) | -0.0035 (11) | 0.0240 (13) | -0.0114 (11) |
| C6 | 0.0477 (15) | 0.0703 (16) | 0.0468 (15) | 0.0002 (12) | 0.0315 (14) | -0.0041 (12) |
| C14 | 0.0455 (15) | 0.0674 (15) | 0.0538 (16) | -0.0046 (12) | 0.0361 (14) | -0.0031 (12) |
| C11 | 0.0479 (15) | 0.0570 (13) | 0.0509 (15) | -0.0084 (12) | 0.0355 (14) | -0.0110 (11) |
| C13 | 0.0386 (14) | 0.0809 (17) | 0.0573 (17) | -0.0073 (13) | 0.0299 (14) | -0.0053 (13) |
| C12 | 0.0424 (15) | 0.0643 (15) | 0.0435 (15) | -0.0053 (12) | 0.0247 (13) | -0.0060 (11) |
| C5 | 0.0528 (17) | 0.100 (2) | 0.0516 (16) | -0.0027 (16) | 0.0381 (15) | -0.0121 (15) |
| C4 | 0.0513 (17) | 0.087 (2) | 0.0610 (18) | 0.0025 (15) | 0.0369 (16) | -0.0217 (15) |
| C3 | 0.0491 (16) | 0.0606 (15) | 0.0614 (17) | 0.0022 (13) | 0.0324 (15) | -0.0135 (13) |
| C7 | 0.0658 (19) | 0.0565 (15) | 0.075 (2) | -0.0007 (13) | 0.0473 (18) | 0.0007 (13) |
| C15 | 0.071 (2) | 0.164 (3) | 0.0525 (19) | -0.016 (2) | 0.0442 (19) | -0.0258 (19) |
| O1 | 0.0668 (12) | 0.0571 (9) | 0.0569 (12) | 0.0121 (9) | 0.0393 (11) | 0.0084 (8) |
| O2 | 0.0360 (9) | 0.0696 (10) | 0.0542 (10) | -0.0035 (8) | 0.0305 (9) | -0.0118 (8) |
| O3 | 0.0606 (12) | 0.0922 (13) | 0.0561 (12) | -0.0179 (10) | 0.0449 (11) | -0.0102 (9) |
| O4 | 0.0531 (12) | 0.1345 (16) | 0.0517 (12) | -0.0218 (11) | 0.0380 (11) | -0.0281 (11) |
| S1 | 0.0400 (4) | 0.0541 (4) | 0.0427 (4) | 0.0021 (3) | 0.0267 (3) | -0.0040 (3) |
| N1 | 0.0450 (12) | 0.0577 (12) | 0.0394 (12) | -0.0091 (9) | 0.0301 (11) | -0.0074 (9) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------|-----------|---------|-----------|
| C1—C6 | 1.388 (3) | C13—H13 | 0.9300 |
| C1—C2 | 1.404 (3) | C12—H12 | 0.9300 |
| C1—S1 | 1.762 (2) | C5—C4 | 1.370 (4) |

| | | | |
|-------------|-------------|---------------|-------------|
| C9—C10 | 1.388 (3) | C5—H5 | 0.9300 |
| C9—C14 | 1.394 (3) | C4—C3 | 1.376 (4) |
| C9—C8 | 1.487 (3) | C4—H4 | 0.9300 |
| C10—C11 | 1.382 (3) | C3—H3 | 0.9300 |
| C10—H10 | 0.9300 | C7—H7A | 0.9600 |
| C8—O3 | 1.213 (3) | C7—H7B | 0.9600 |
| C8—N1 | 1.387 (3) | C7—H7C | 0.9600 |
| C2—C3 | 1.400 (3) | C15—O4 | 1.431 (3) |
| C2—C7 | 1.509 (3) | C15—H15A | 0.9600 |
| C6—C5 | 1.393 (3) | C15—H15B | 0.9600 |
| C6—H6 | 0.9300 | C15—H15C | 0.9600 |
| C14—C13 | 1.363 (3) | O1—S1 | 1.4232 (16) |
| C14—H14 | 0.9300 | O2—S1 | 1.4391 (16) |
| C11—O4 | 1.360 (3) | S1—N1 | 1.666 (2) |
| C11—C12 | 1.385 (3) | N1—HN1 | 0.79 (2) |
| C13—C12 | 1.386 (3) | | |
| | | | |
| C6—C1—C2 | 122.0 (2) | C4—C5—H5 | 120.2 |
| C6—C1—S1 | 116.49 (18) | C6—C5—H5 | 120.2 |
| C2—C1—S1 | 121.48 (17) | C5—C4—C3 | 120.7 (2) |
| C10—C9—C14 | 119.7 (2) | C5—C4—H4 | 119.6 |
| C10—C9—C8 | 123.6 (2) | C3—C4—H4 | 119.6 |
| C14—C9—C8 | 116.6 (2) | C4—C3—C2 | 121.9 (2) |
| C11—C10—C9 | 120.0 (2) | C4—C3—H3 | 119.1 |
| C11—C10—H10 | 120.0 | C2—C3—H3 | 119.1 |
| C9—C10—H10 | 120.0 | C2—C7—H7A | 109.5 |
| O3—C8—N1 | 120.2 (2) | C2—C7—H7B | 109.5 |
| O3—C8—C9 | 122.5 (2) | H7A—C7—H7B | 109.5 |
| N1—C8—C9 | 117.3 (2) | C2—C7—H7C | 109.5 |
| C3—C2—C1 | 116.3 (2) | H7A—C7—H7C | 109.5 |
| C3—C2—C7 | 119.0 (2) | H7B—C7—H7C | 109.5 |
| C1—C2—C7 | 124.7 (2) | O4—C15—H15A | 109.5 |
| C1—C6—C5 | 119.4 (2) | O4—C15—H15B | 109.5 |
| C1—C6—H6 | 120.3 | H15A—C15—H15B | 109.5 |
| C5—C6—H6 | 120.3 | O4—C15—H15C | 109.5 |
| C13—C14—C9 | 119.5 (2) | H15A—C15—H15C | 109.5 |
| C13—C14—H14 | 120.2 | H15B—C15—H15C | 109.5 |
| C9—C14—H14 | 120.2 | C11—O4—C15 | 117.5 (2) |
| O4—C11—C10 | 115.8 (2) | O1—S1—O2 | 118.18 (11) |
| O4—C11—C12 | 124.0 (2) | O1—S1—N1 | 108.93 (10) |
| C10—C11—C12 | 120.2 (2) | O2—S1—N1 | 103.29 (10) |
| C14—C13—C12 | 121.4 (2) | O1—S1—C1 | 109.21 (11) |
| C14—C13—H13 | 119.3 | O2—S1—C1 | 110.47 (10) |
| C12—C13—H13 | 119.3 | N1—S1—C1 | 105.95 (11) |
| C11—C12—C13 | 119.1 (2) | C8—N1—S1 | 122.61 (17) |
| C11—C12—H12 | 120.4 | C8—N1—HN1 | 120.7 (19) |
| C13—C12—H12 | 120.4 | S1—N1—HN1 | 116.5 (19) |
| C4—C5—C6 | 119.6 (2) | | |

| | | | |
|-----------------|--------------|----------------|--------------|
| C14—C9—C10—C11 | 0.0 (3) | C5—C4—C3—C2 | -0.1 (4) |
| C8—C9—C10—C11 | -179.7 (2) | C1—C2—C3—C4 | 0.1 (4) |
| C10—C9—C8—O3 | 161.3 (2) | C7—C2—C3—C4 | 179.1 (2) |
| C14—C9—C8—O3 | -18.4 (3) | C10—C11—O4—C15 | 176.7 (2) |
| C10—C9—C8—N1 | -17.9 (3) | C12—C11—O4—C15 | -2.7 (4) |
| C14—C9—C8—N1 | 162.4 (2) | O2—O2—S1—O1 | 0.00 (5) |
| C6—C1—C2—C3 | 0.0 (3) | O2—O2—S1—N1 | 0.00 (6) |
| S1—C1—C2—C3 | 178.99 (18) | O2—O2—S1—C1 | 0.00 (4) |
| C6—C1—C2—C7 | -178.9 (2) | C6—C1—S1—O1 | 10.5 (2) |
| S1—C1—C2—C7 | 0.1 (3) | C2—C1—S1—O1 | -168.48 (18) |
| C2—C1—C6—C5 | -0.2 (4) | C6—C1—S1—O2 | 142.13 (18) |
| S1—C1—C6—C5 | -179.17 (18) | C2—C1—S1—O2 | -36.9 (2) |
| C10—C9—C14—C13 | 0.2 (3) | C6—C1—S1—O2 | 142.13 (18) |
| C8—C9—C14—C13 | 179.9 (2) | C2—C1—S1—O2 | -36.9 (2) |
| C9—C10—C11—O4 | -179.6 (2) | C6—C1—S1—N1 | -106.65 (19) |
| C9—C10—C11—C12 | -0.1 (3) | C2—C1—S1—N1 | 74.3 (2) |
| C9—C14—C13—C12 | -0.2 (4) | O3—C8—N1—S1 | -3.9 (3) |
| O4—C11—C12—C13 | 179.5 (2) | C9—C8—N1—S1 | 175.28 (15) |
| C10—C11—C12—C13 | 0.1 (4) | O1—S1—N1—C8 | -54.9 (2) |
| C14—C13—C12—C11 | 0.1 (4) | O2—S1—N1—C8 | 178.66 (18) |
| C1—C6—C5—C4 | 0.2 (4) | O2—S1—N1—C8 | 178.66 (18) |
| C6—C5—C4—C3 | 0.0 (4) | C1—S1—N1—C8 | 62.5 (2) |

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|------------------------------|----------|----------|-----------|---------|
| N1—HN1···O2 ⁱ | 0.80 (3) | 2.15 (4) | 2.929 (4) | 166 |
| C3—H3···O3 ⁱⁱ | 0.93 | 2.60 | 3.463 (3) | 155 |
| C10—H10···O2 ⁱ | 0.93 | 2.60 | 3.404 (3) | 145 |
| C15—H15B···O3 ⁱⁱⁱ | 0.96 | 2.36 | 3.323 (3) | 178 |
| C6—H6···O1 | 0.93 | 2.46 | 2.861 (4) | 106 |

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $x, y-1, z$; (iii) $x, -y+2, z+1/2$.